

Wiener Integration for Quantum Systems: A Unified Approach to the Feynman-Kac formula *

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Abstract

A generalized Feynman–Kac formula based on the Wiener measure is presented. Within the setting of a quantum particle in an electromagnetic field it yields the standard Feynman–Kac formula for the corresponding Schrödinger semigroup. In this case rigorous criteria for its validity are compiled. Finally, phase-space path-integral representations for more general quantum Hamiltonians are derived. These representations rely on a generalized Lie–Trotter formula which takes care of the operator-ordering multiplicity, but in general is not related to a path measure.

Actually, in the Wiener integral the things are much simpler. [46]

1 The Feynman–Kac formula, revisited

More than seventy years of Wiener’s path integration have been most gratifying for both mathematicians and theoretical physicists. Originally constructed as a mathematical model for the phenomenon of Brownian motion, it nowadays plays a major rôle also in polymer and quantum physics, and still is fundamental to the theory of general stochastic processes [39]. The importance of Wiener’s measure [45] for quantum physics became clear soon after Feynman’s stimulating paper [16] when Kac [24, 25] identified it as the key to a probabilistic representation of Schrödinger semigroups, these days called the Feynman–Kac formula [42, 20, 40].

In this section we intend to survey essentials of this formula and some of its relatives. In doing so, we leave aside most technicalities and subtleties which we believe to be of secondary importance for applications, in particular when they tend to obscure the simplicity of the underlying ideas.

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1.1 The Wiener measure and stochastic integrals

The standard *Wiener measure* Dw is a certain probability distribution on the space of continuous paths $\{w : \mathbb{R}_+ \rightarrow \mathbb{R}^d, s \mapsto w(s)\}$ from the positive half-line $\mathbb{R}_+ := [0, \infty[$ into d -dimensional Euclidean space \mathbb{R}^d which start at the origin, $w(0) = 0$. It is uniquely determined and well-defined by the following properties:

- i) Dw is a Gaussian probability measure.
- ii) Its first and second moments are

$$\int Dw w_j(s) = 0, \quad \int Dw w_j(r) w_k(s) = \delta_{jk} \min(r, s). \quad (1)$$

Here and in the following indices j, k, \dots denumerate the components of d -component quantities, $x \cdot y := \sum_{j=1}^d x_j y_j$ denotes the standard scalar product of two such quantities, and the usual convention $x^2 := x \cdot x$ is adopted. Kronecker's delta in (1) expresses the stochastic independence of different components of w . A one-line characterization of Dw , equivalent to i) and ii), is given by its (functional) Fourier transform

$$\int Dw \exp \left\{ -i \int_0^\infty ds w(s) \cdot f(s) \right\} = \exp \left\{ -\frac{1}{2} \int_0^\infty dr \int_0^\infty ds \min(r, s) f(r) \cdot f(s) \right\} \quad (2)$$

where $f : \mathbb{R}_+ \rightarrow \mathbb{R}^d$ is any d -component function with compact support in the half-line \mathbb{R}_+ .

Whenever the Wiener measure $Dw = \prod_{1 \leq j \leq d} Dw_j$ is applicable, its advantages over lattice or time-slicing prescriptions for path integration can hardly be overestimated. Since Dw is a positive, countably additive and normalized measure, the powerful machinery of general integration and probability theory [29, 7] is at hand for the computation or estimation of Wiener integrals $\int Dw F(w)$, where F is a functional of the paths. The importance of Dw for integration in infinite-dimensional path space $(\mathbb{R}^d)^{\mathbb{R}_+}$ is similar to that of Lebesgue's measure $dx = \prod_{1 \leq j \leq d} dx_j$ for 'ordinary' integration in \mathbb{R}^d .

For an intuitive understanding of Dw it is sometimes helpful to think of it as an infinite-dimensional Lebesgue measure with Gaussian weight

$$\prod_{\substack{0 \leq s \\ 1 \leq j \leq d}} \left(\frac{dw_j(s)}{\sqrt{2\pi\Delta s}} \exp \left\{ -\frac{\Delta s}{2} \dot{w}_j(s)^2 \right\} \right) \quad (3)$$

in the limit $\Delta s \downarrow 0$. Strictly speaking, expression (3) is meaningless because there is no translational invariant measure in infinite dimensions. In addition, *Wiener paths* almost surely have no time derivative $\dot{w} := \frac{d}{ds} w$ for any s and hence are not of bounded variation on any compact interval $[0, t]$, see e.g. [7]. Nevertheless, the concept of *stochastic integrals* allows to give precise meaning in a suitable probabilistic sense to (line) integrals of the form

$$\int_0^t ds \dot{w}(s) \cdot g(w(s), s), \quad t \geq 0 \quad (4)$$

for a wide class of functions $g : \mathbb{R}^d \times \mathbb{R}_+ \rightarrow \mathbb{R}^d$. In principle, there is a huge

multiplicity of rigorously definable candidates [39, p. 136] for (4). As a rule however, literature [5, 33, 39] discusses at most a one-parameter subclass of stochastic integrals, denoted by us as

$$\textcircled{\alpha} \int_0^t dw(s) \cdot g(w(s), s), \quad \alpha \in [0, 1]. \quad (5)$$

While probabilists usually use $\alpha = 0$ corresponding to Itô's original proposal, we will here follow Stratonovich in choosing $\alpha = 1/2$ for the interpretation of (4), so that the rules of ordinary calculus in the sense of Newton and Leibniz formally apply. By the conversion formula [33, p. 113] [39, p. 136]

$$\int_0^t ds \dot{w}(s) \cdot g(w(s), s) = \textcircled{\alpha} \int_0^t dw(s) \cdot g(w(s), s) + \left(\frac{1}{2} - \alpha\right) \int_0^t ds (\nabla \cdot g)(w(s), s) \quad (6)$$

the Stratonovich stochastic integral is related to the α -stochastic integral. Note that the second integral on the right-hand side containing the divergence of g is understood in the Lebesgue sense because of the continuity of Wiener paths. Stochastic integrals can also be defined for functions $(w, s) \mapsto g(w, s)$ which in their first argument may depend on the whole history $\{w(r)\}_{r \leq s}$ of the path up to the time value of the second argument [5, 33, 39]. Such non-anticipating functions might take values in \mathbb{R}^d , in a Hilbert space or even in a set of Hilbert-space operators [20].

As a simple application of the preceding discussion one obtains

$$\int Dw \exp \left\{ -i \int_0^\infty ds \dot{w}(s) \cdot f(s) \right\} = \exp \left\{ -\frac{1}{2} \int_0^\infty ds f(s)^2 \right\} \quad (7)$$

for compactly supported f . This follows from (formal) integration by parts, equation (2) and the representation $\delta(r - s) = \frac{\partial^2}{\partial r \partial s} \min(r, s)$ of Dirac's delta function. In analogy to (2), equation (7) may serve as a one-line characterization of d -component *Gaussian white noise*.

1.2 A generalization of the Feynman–Kac formula

The main purpose of this subsection is to extend equation (7) to certain operator-valued functions f . Accordingly, let $\hat{A} = (\hat{A}_1, \dots, \hat{A}_d)$ be a d -component operator acting on some separable Hilbert space \mathcal{H} . Moreover, let \hat{B} be another operator and $\hat{1}$ the identity on \mathcal{H} . For notational simplicity we will assume that \hat{A} and \hat{B} are time-independent, the extension to the time-dependent case being straightforward. Finally, let $\hat{T}_t(w)$ be the operator solving the linear *stochastic integral equation*

$$\hat{T}_t = \hat{1} - i \int_0^t ds \dot{w}(s) \cdot \hat{A} \hat{T}_s - \hat{B} \int_0^t ds \hat{T}_s \quad (8)$$

which is the precise formulation of the linear (Stratonovich) stochastic differential equation

$$\frac{d}{dt} \hat{T}_t = -i (\dot{w}(t) \cdot \hat{A} - i \hat{B}) \hat{T}_t, \quad \hat{T}_0 = \hat{1}. \quad (9)$$

In analogy to quantum dynamics with explicitly time-dependent Hamiltonians the

solution $\widehat{T}_t(w)$ can be obtained by iterating (8)

$$\begin{aligned} \widehat{T}_t(w) &= \hat{1} + \sum_{n=1}^{\infty} (-i)^n \int_0^t ds_n \left(\dot{w}(s_n) \cdot \widehat{A} - i\widehat{B} \right) \int_0^{s_n} ds_{n-1} \\ &\quad \times \left(\dot{w}(s_{n-1}) \cdot \widehat{A} - i\widehat{B} \right) \cdots \int_0^{s_2} ds_1 \left(\dot{w}(s_1) \cdot \widehat{A} - i\widehat{B} \right) \end{aligned} \quad (10)$$

$$=: \overleftarrow{\exp} \left\{ -i \int_0^t ds \left(\dot{w}(s) \cdot \widehat{A} - i\widehat{B} \right) \right\} \quad (11)$$

which defines Dyson's time-ordered exponential function $\overleftarrow{\exp}$, also known as product integral.

Now we are prepared to state a *generalized Feynman–Kac formula*

$$\boxed{\int Dw \widehat{T}_t(w) = \exp \left\{ -t \left(\frac{1}{2} \widehat{A}^2 + \widehat{B} \right) \right\}}. \quad (12)$$

As we will see in the next subsection, the standard Feynman–Kac formula follows by a suitable choice of \mathcal{H} , \widehat{A} and \widehat{B} . A heuristic argument for the validity of (12) goes as follows: In the presence of time-ordering, \widehat{B} and all components of \widehat{A} may be treated as pairwise commuting [17, 28], so that a formal application of (7) to (10) with $f(s) = \Theta(t-s)\widehat{A}$ gives the desired result. Here Θ stands for Heaviside's unit-step function.

A more convincing argument for (12) proceeds in two steps. First consider the case of vanishing \widehat{B} . Wiener integrating both sides of (8) and supposing

$$\left\langle \int_0^t ds \dot{w}_j(s) \widehat{T}_s \right\rangle = -\frac{i}{2} \widehat{A}_j \left\langle \int_0^t ds \widehat{T}_s \right\rangle, \quad (13)$$

where for convenience the notation $\langle \cdot \rangle := \int Dw (\cdot)$ is introduced, yields the integral equation

$$\langle \widehat{T}_t \rangle = \hat{1} - \frac{1}{2} \widehat{A}^2 \int_0^t ds \langle \widehat{T}_s \rangle \quad (14)$$

which, in turn, gives $\langle \widehat{T}_t \rangle = \exp\{-\frac{t}{2} \widehat{A}^2\}$. Equation (13) follows from integration by parts with respect to Dw using its Gaussian nature (cf. [41, p. 32 and solution of exercise 1.8.22]) and the convention $\Theta(0) := 1/2$ corresponding to the Stratonovich interpretation. For a rigorous proof of (13) one should use Malliavin's stochastic variational calculus [37, 32]. Clearly, if the components of \widehat{A} commute, time ordering can be dropped, so that the result is obtained directly from $\widehat{T}_t(w) = \exp(-i w(t) \cdot \widehat{A})$ and (2).

The case $\widehat{B} \neq \widehat{0}$ will now be treated in the second step by a perturbative argument in the spirit of Kac's original proof for the standard Feynman–Kac formula (see [25, 42, 40]). For this purpose, we define

$$\widehat{U}_t(w) := \overleftarrow{\exp} \left\{ -i \int_0^t ds \dot{w}(s) \cdot \widehat{A} \right\} \quad (15)$$

and

$$\widehat{S}_t(w) := \overleftarrow{\exp} \left\{ - \int_0^t ds \left(\widehat{U}_s(w) \right)^{-1} \widehat{B} \widehat{U}_s(w) \right\} \quad (16)$$

$$= \widehat{1} - \int_0^t ds \left(\widehat{U}_s(w) \right)^{-1} \widehat{B} \widehat{U}_s(w) \widehat{S}_s(w). \quad (17)$$

Then, according to standard time-dependent perturbation theory

$$\widehat{T}_t = \widehat{U}_t \widehat{S}_t = \widehat{U}_t - \int_0^t ds \widehat{U}_t \widehat{U}_s^{-1} \widehat{B} \widehat{T}_s. \quad (18)$$

We now Wiener integrate both sides, assume the identity

$$\langle \widehat{U}_t \widehat{U}_s^{-1} \widehat{B} \widehat{T}_s \rangle = \langle \widehat{U}_{t-s} \rangle \widehat{B} \langle \widehat{T}_s \rangle \quad (19)$$

and recall $\langle \widehat{U}_t \rangle = \exp \left\{ -\frac{t}{2} \widehat{A}^2 \right\}$ from the first step to obtain the Duhamel-type of integral equation

$$\langle \widehat{T}_t \rangle = \exp \left\{ -\frac{t}{2} \widehat{A}^2 \right\} - \int_0^t ds \exp \left\{ -\frac{t-s}{2} \widehat{A}^2 \right\} \widehat{B} \langle \widehat{T}_s \rangle. \quad (20)$$

This implies the initial-value problem

$$\frac{d}{dt} \langle \widehat{T}_t \rangle = - \left(\frac{1}{2} \widehat{A}^2 + \widehat{B} \right) \langle \widehat{T}_t \rangle, \quad \langle \widehat{T}_0 \rangle = \widehat{1} \quad (21)$$

which finally gives (12). The claimed stochastic independence underlying (19) is basically due to the Markov property of Dw and the fact that Wiener paths start continually afresh [42, 7].

We conclude this subsection with four remarks:

- Clearly, the Markov property of the Wiener measure Dw is responsible for the emergence of a *one-parameter operator semigroup* on the right-hand side of the generalized Feynman-Kac formula (12). The Gaussian nature of Dw causes (the negative of) its generator $\frac{1}{2} \widehat{A}^2 + \widehat{B}$ to be quadratic in \widehat{A} . If \widehat{A} and \widehat{B} are Hermitian, the left-hand side manifestly is, because Dw does not change under reflection $w(s) \mapsto -w(s)$.
- Conversely, reading (12) from right to left may be viewed as uncompleting squares of operators in an exponent by *Gaussian linearization*. It is therefore closely related to the so-called Hubbard-Stratonovich trick, widely used in different branches of theoretical physics. For applications to certain many-body systems see the surveys [34, 27] and references therein. To our knowledge, so far mainly the case of commuting \widehat{A} -components has been considered in this context. There is also a noteworthy similarity to Feynman's disentangling formalism [17, 35].

- A simple corollary of (12) for $d = 2$, namely

$$\begin{aligned} & \int Dw \overleftarrow{\exp} \left\{ -i \int_0^t ds \left[\left(\dot{w}_1(s) + i \dot{w}_2(s) \right) \widehat{A}_+ + \left(\dot{w}_1(s) - i \dot{w}_2(s) \right) \widehat{A}_- - i \widehat{B} \right] \right\} \\ &= \exp \left\{ -t \left(\widehat{A}_+ \widehat{A}_- + \widehat{A}_- \widehat{A}_+ + \widehat{B} \right) \right\}, \end{aligned} \quad (22)$$

follows from the non-commutative extension

$$\hat{A}_+ \hat{A}_- + \hat{A}_- \hat{A}_+ = \frac{1}{2} (\hat{A}_+ + \hat{A}_-)^2 - \frac{1}{2} (\hat{A}_+ - \hat{A}_-)^2 \quad (23)$$

of the binomial formula for a pair of operators \hat{A}_+ and \hat{A}_- . This shows that one can also linearize symmetrized products of two, in general non-commuting operators.

- In case of an infinite-dimensional Hilbert space \mathcal{H} the arguments and computations in our derivation are rather formal, unless one specifies a class of admissible operators \hat{A} and \hat{B} which is sufficiently wide to be of interest for applications. In particular, domain questions require additional efforts. See, for example, subsection 1.4 below.

1.3 The standard Feynman–Kac formula

In this subsection we specialize to the usual setting for non-relativistic quantum mechanics of an electrically charged point mass in \mathbb{R}^d without internal degrees of freedom. Consequently, let $L^2(\mathbb{R}^d)$ be the Hilbert space of complex-valued functions $\psi : \mathbb{R}^d \rightarrow \mathbb{C}, q \mapsto \psi(q)$, which are square-integrable with respect to the Lebesgue measure dq . Consider now a vector potential $a : \mathbb{R}^d \rightarrow \mathbb{R}^d$ and a scalar potential $v : \mathbb{R}^d \rightarrow \mathbb{R}$, both sufficiently well-behaved. They give rise to a standard Hamiltonian, or Schrödinger operator, $\hat{H} := \frac{1}{2} (\hat{p} - a(\hat{q}))^2 + v(\hat{q})$ on $L^2(\mathbb{R}^d)$ with magnetic field $b_{jk} := \frac{\partial a_j}{\partial q_k} - \frac{\partial a_k}{\partial q_j}$. Here \hat{p} and \hat{q} denote the usual self-adjoint momentum and position operators. For notational simplicity, we choose units such that Planck's constant \hbar , the mass and the charge of the particle are all unity.

Then the *standard Feynman–Kac formula* with a vector potential reads

$$\boxed{e^{-t\hat{H}} = \int Dw e^{-iw(t) \cdot \hat{p}} \exp \left\{ i \int_0^t ds \dot{w}(s) \cdot a(\hat{q} + w(s)) - \int_0^t ds v(\hat{q} + w(s)) \right\}} \quad (24)$$

In fact, it is a special case of (12) for the choice $\mathcal{H} = L^2(\mathbb{R}^d)$, $\hat{A} = \hat{p} - a(\hat{q})$ and $\hat{B} = v(\hat{q})$. This follows from the first equation in (18) and the identity

$$\widehat{U}_t(w) = \overleftarrow{\exp} \left\{ -i \int_0^t ds \dot{w}(s) \cdot (\hat{p} - a(\hat{q})) \right\} \quad (25)$$

$$= e^{-iw(t) \cdot \hat{p}} \exp \left\{ i \int_0^t ds \dot{w}(s) \cdot a(\hat{q} + w(s)) \right\} \quad (26)$$

which is again understood with the help of time-dependent perturbation theory in combination with the fact that the time-dependent operator components

$$e^{iw(s) \cdot \hat{p}} a_j(\hat{q}) e^{-iw(s) \cdot \hat{p}} = a_j(\hat{q} + w(s)) \quad (27)$$

commute for all values of j and s . The specialization is completed by observing a similar shift-identity for the scalar potential in $\hat{S}_t(w)$.

Several remarks apply:

- The Wiener integral has managed to completely disentangle the non-commuting operators \hat{p} and \hat{q} in the *Schrödinger semigroup* $\exp(-t\hat{H})$. The standard Feynman–Kac formula in its basis-independent version (24) has been presented before (cf. e.g. [19, 1, 9]). Apart from mathematical subtleties, this abstract way of looking at the Feynman–Kac formula extracts its essential ingredients and is often a convenient starting point for further manipulations.
- The Stratonovich stochastic integral in (24) may be replaced by the corresponding α -stochastic integral using the conversion formula (6). The resulting formula might be called the *Feynman–Kac- α formula* extending a terminology introduced by Simon [42]. The correct unitary transformation $e^{-t\hat{H}} \mapsto e^{i\chi(\hat{q})}e^{-t\hat{H}}e^{-i\chi(\hat{q})}$ under a change of gauge $a \mapsto a + \nabla\chi$ is most easily obtained from (24) by using the rules of ordinary calculus.
- By applying both sides of (24) to a wave function $\psi \in L^2(\mathbb{R}^d)$ it is straightforward to derive the usual probabilistic expression for its image $\exp(-t\hat{H})\psi$ under the Schrödinger semigroup (cf. [42, eqs. (6.8) and (15.1)])

$$\begin{aligned} (e^{-t\hat{H}}\psi)(q) &= \int Dw \exp \left\{ -i \int_0^t ds \dot{w}(s) \cdot a(q + w(s)) \right\} \\ &\quad \times \exp \left\{ - \int_0^t ds v(q + w(s)) \right\} \psi(q + w(t)). \end{aligned} \quad (28)$$

This can be rewritten as

$$(e^{-t\hat{H}}\psi)(q) = \int dq' \langle q | e^{-t\hat{H}} | q' \rangle \psi(q') \quad (29)$$

where the Euclidean propagator, that is, the position representation of the semigroup, is given by

$$\begin{aligned} \langle q | e^{-t\hat{H}} | q' \rangle &= \int Dw \delta(w(t) + q - q') \exp \left\{ -i \int_0^t ds \dot{w}(s) \cdot a(q + w(s)) \right\} \\ &\quad \times \exp \left\{ - \int_0^t ds v(q + w(s)) \right\}. \end{aligned} \quad (30)$$

Here, due to the presence of the delta function, effectively only those Wiener paths contribute which pass through $q' - q$ at time t . One may also integrate over the rigidly shifted paths $s \mapsto w(s) + q$ which start at q and pass through q' at time t .

- As a final point in this subsection, we mention a close relative of (28), the probabilistic representation of the unitary time evolution

$$\begin{aligned} (e^{-it\hat{H}}\psi)(q) &= \int Dw \exp \left\{ -i\sqrt{i} \int_0^t ds \dot{w}(s) \cdot a(q + \sqrt{i}w(s)) \right\} \\ &\quad \times \exp \left\{ -i \int_0^t ds v(q + \sqrt{i}w(s)) \right\} \psi(q + \sqrt{i}w(t)). \end{aligned} \quad (31)$$

It is obtained analogously to (24) and (28) by choosing $\hat{A} = \sqrt{i}(\hat{p} - a(\hat{q}))$ and $\hat{B} = iv(\hat{q})$ in (12). Its validity obviously requires some analyticity assumptions on the potentials and the (initial) wavefunction. For rigorous discussions of (31) (in the case $a = 0$), see [21, 6] and the book [22] on a related theme.

1.4 On the validity of the standard Feynman–Kac formula

Equations (28) and (30) are the most popular versions of the Feynman–Kac formula. It is therefore fortunate that there is a wealth of information about the conditions under which they are rigorously valid. We take the opportunity to recall some rather weak assumptions on the potentials a and v which are sufficient [42, 43, 3, 12, 10]. To this end, let $L_{loc}^p(\mathbb{R}^d)$, $p \in [1, \infty[$, denote the space of complex-valued functions $\varphi : \mathbb{R}^d \rightarrow \mathbb{C}$ with $\int_{\Lambda} d\mathbf{q} |\varphi(\mathbf{q})|^p < \infty$ for all compact $\Lambda \subset \mathbb{R}^d$. Let $v_{\pm}(\mathbf{q}) := \sup\{0, \pm v(\mathbf{q})\}$ be the positive and negative part of the scalar potential $v = v_+ - v_-$.

In a first step we show the existence of the Wiener integral in (28) for $a = 0$ and v_- belonging to the Katô class $\mathcal{K}(\mathbb{R}^d)$, that is, $\lim_{t \downarrow 0} \kappa_t(v_-) = 0$ where

$$\kappa_t(u) := \sup_{x \in \mathbb{R}^d} \int Dw \int_0^t ds |u(x + w(s))| = \sup_{x \in \mathbb{R}^d} \int_0^t ds \left(e^{-s\hat{p}^2/2} |u| \right)(x). \quad (32)$$

Due to the Markov property of Dw one may assume without loss of generality $t > 0$ sufficiently small, so that $\kappa_t(v_-) < 1/2$. Then the following estimate holds

$$\left| \int Dw \exp \left\{ - \int_0^t ds v(q + w(s)) \right\} \psi(q + w(t)) \right|^2 \leq \frac{\int dx |\psi(x)|^2}{(2\pi t)^{d/2} (1 - 2\kappa_t(v_-))}. \quad (33)$$

Its proof starts from employing the Cauchy–Schwarz–Bunyakovski inequality

$$|\langle M_t(q, v) \psi(q + w(t)) \rangle|^2 \leq \langle M_t(q, 2v) \rangle \langle |\psi(q + w(t))|^2 \rangle \quad (34)$$

with respect to Dw , where we have introduced the (multiplicative) functional

$$M_t(q, v) := \exp \left\{ - \int_0^t ds v(q + w(s)) \right\}. \quad (35)$$

While the second factor on the right-hand side of (34) is easily seen not to exceed $\int dx |\psi(x)|^2 / (2\pi t)^{d/2} < \infty$, the first factor is estimated using $-v \leq v_-$ and *Khas'minskii's Lemma* [26, 3, 43] $\langle M_t(q, -v_-) \rangle \leq (1 - \kappa_t(v_-))^{-1}$.

Now turning on the vector potential a , the conditions $a^2, \nabla \cdot a \in L_{loc}^1(\mathbb{R}^d)$ are sufficient for the existence of the Stratonovich stochastic integral in (28) (and hence of the corresponding α -stochastic integral for arbitrary α). Since it appears there as the phase of a complex number of absolute value one, the Wiener integral in (28) remains bounded from above by the right-hand side of (33). In other words, the diamagnetic inequality [42] has extended (33) to non-vanishing a .

In order to guarantee equality (28), at least for Lebesgue-every q , one needs a condition on v_+ , in addition to the above assumptions on a and v_- . For example, if $v_+ \in L_{loc}^1(\mathbb{R}^d)$ the Hamiltonian \widehat{H} can be precisely defined in the sense of quadratic forms as a self-adjoint operator on $L^2(\mathbb{R}^d)$ bounded from below and (28) holds. Under the stronger assumptions $v_- \in \mathcal{K}(\mathbb{R}^d) \cap L_{loc}^2(\mathbb{R}^d)$ and $v_+, a^2, \nabla \cdot a \in L_{loc}^2(\mathbb{R}^d)$ the space of arbitrarily often differentiable complex-valued functions with compact support, $C_0^\infty(\mathbb{R}^d)$, can even be identified as an operator domain of essential self-adjointness.

Pointwise validity of (28) is assured by the assumptions $v_- \in \mathcal{K}(\mathbb{R}^d)$ and $v_+, a^2, \nabla \cdot a \in \mathcal{K}_{loc}(\mathbb{R}^d) \subset L^1_{loc}(\mathbb{R}^d)$, where by definition $u \in \mathcal{K}_{loc}(\mathbb{R}^d)$ if $u\varphi \in \mathcal{K}(\mathbb{R}^d)$ for all $\varphi \in C_0^\infty(\mathbb{R}^d)$. Under these assumptions the semigroup $\exp(-t\widehat{H})$ maps $L^2(\mathbb{R}^d)$ into its subspace of functions which are continuous (and bounded). As a consequence, both sides in (28) are continuous and hence coincide for all q . Even more, the semigroup possesses then for each $t > 0$ an integral kernel $(q, q') \mapsto \langle q | \exp(-t\widehat{H}) | q' \rangle$ which is jointly continuous in (t, q, q') for $t > 0$ and $q, q' \in \mathbb{R}^d$. It can be expressed by the right-hand side of (30), provided the delta function is understood in the sense of Donsker or Hida (see e.g. [22]), or the integration $\int Dw \delta(w(t) + q - q')(\cdot)$ is interpreted as a short-hand for averaging with respect to the Brownian bridge [42, 40, 10] from $(0, q)$ to (t, q') .

An important example of a scalar potential, for which (28) holds pointwise and the right-hand side of (30) defines the corresponding continuous integral kernel, is the inverse-distance potential $v(q) = -\gamma/|q|$, $\gamma \in \mathbb{R}$, for $d \geq 2$. Complications in the case $d = 1$ are treated in [18].

2 Phase-space path integrals for non-standard Hamiltonians

Phase-space path integrals serve to provide a generalization of the standard Feynman-Kac formula to non-standard Hamiltonians on $L^2(\mathbb{R}^d)$, that is, Hamiltonians more general than $\widehat{H} = \frac{1}{2}(\hat{p} - a(\hat{q}))^2 + v(\hat{q})$. This idea dates back to Feynman [17] and is still used in quantum physics (see, e. g. [44, Ch. 9]). Any attempt to put it on safer grounds has to face the problem that there is no unique correspondence between Hilbert-space operators and phase-space functions. Until now the most popular method to give meaning to Feynman's heuristic idea of phase-space path integrals employs lattice or time-slicing prescriptions. Since the seventies it is well-known [4, 14, 31, 8, 30, 38] that this method reflects the above non-uniqueness by a multiplicity of prescriptions, each linked to a particular way of choosing the order for the factors in a product of non-commuting operators. In our opinion the most systematic way to keep track of this is to proceed via linear phase-space representations (also known as symbol-calculus in the theory of pseudo-differential operators) and a generalized Lie-Trotter formula. In this section we are going to briefly summarize such a procedure, restricting ourselves for clarity to certain one-parameter subclasses among phase-space representations and corresponding lattice prescriptions.

Following [31] we associate with a given Hamilton operator \widehat{H} on $L^2(\mathbb{R}^d)$ a one-parameter family of *symbols*, that is, functions on classical phase space $\mathbb{R}^d \times \mathbb{R}^d$ defined by

$$H_\alpha(p, q) := \int dx e^{ip \cdot x} \langle q - (1 - \alpha)x | \widehat{H} | q + \alpha x \rangle, \quad \alpha \in [0, 1]. \quad (36)$$

For each fixed α the linear mapping $\widehat{H} \mapsto H_\alpha$ of Hilbert-space operators to phase-

space functions can be inverted according to $\{H_\alpha(\hat{p}, \hat{q})\}_\alpha = \widehat{H}$. Here the mapping

$$H \mapsto \{H(\hat{p}, \hat{q})\}_\alpha := \int \frac{dp dq}{(2\pi)^d} e^{i(\hat{p}-p) \cdot q} H(p, \hat{q} + \alpha q). \quad (37)$$

is a quantization or *operator-ordering scheme* [2] for phase-space functions H which gives for $\alpha = 0, 1/2, 1$ anti-standard (\hat{p} left of \hat{q}), Weyl–Wigner (totally symmetrized) and standard (\hat{p} right of \hat{q}) ordering, respectively. A nice illustration is already provided by the example of a standard Hamiltonian

$$\widehat{H} = \frac{1}{2} (\hat{p} - a(\hat{q}))^2 + v(\hat{q}) \quad (38)$$

$$H_\alpha(p, q) = \frac{1}{2} (p - a(q))^2 + i \left(\alpha - \frac{1}{2} \right) (\nabla \cdot a)(q) + v(q). \quad (39)$$

Note that the α -symbol H_α is real for all Hermitian \widehat{H} if and only if $\alpha = 1/2$.

We associate with a given \widehat{H} for each α the operator-valued function

$$\widehat{R}_\alpha(t) := \int \frac{dp dq}{(2\pi)^d} e^{i(\hat{p}-p) \cdot q} \exp \{-t H_\alpha(p, \hat{q} + \alpha q)\}, \quad t \geq 0. \quad (40)$$

It provides a short-time approximation to the semigroup $\exp(-t\widehat{H})$ in the sense that

$$\widehat{R}_\alpha(0) = \hat{1}, \quad \dot{\widehat{R}}_\alpha(0) := \left. \frac{d}{dt} \widehat{R}_\alpha(t) \right|_{t=0} = -\widehat{H}. \quad (41)$$

The idea now is to represent $\exp(-t\widehat{H})$ for arbitrary $t \geq 0$ as $[\widehat{R}_\alpha(\frac{t}{n})]^n$ in the limit $n \rightarrow \infty$ by writing

$$\exp \{-t\widehat{H}\} = \exp \{t \dot{\widehat{R}}_\alpha(0)\} = \lim_{n \rightarrow \infty} [\widehat{R}_\alpha(\frac{t}{n})]^n \quad (42)$$

$$\begin{aligned} &= \lim_{n \rightarrow \infty} \int \frac{dp^{(n)} dq^{(n)}}{(2\pi)^d} \cdots \int \frac{dp^{(1)} dq^{(1)}}{(2\pi)^d} e^{-iq^{(n)} \cdot \hat{p}} \\ &\quad \times \exp \left\{ \sum_{\nu=1}^n \left[ip^{(\nu)} \cdot (q^{(\nu)} - q^{(\nu-1)}) - \frac{t}{n} H_\alpha(p^{(\nu)}, \hat{q} + q^{(\nu, \alpha)}) \right] \right\} \end{aligned} \quad (43)$$

where $q^{(0)} := 0$ and the so-called α -point between $q^{(\nu)}$ and $q^{(\nu-1)}$ is defined as $q^{(\nu, \alpha)} := \alpha q^{(\nu)} + (1 - \alpha) q^{(\nu-1)}$. It is customary and mnemonically convenient to use a continuum notation for the right-hand side so that

$$e^{-t\widehat{H}} = \int_\alpha \mathcal{D}\eta \mathcal{D}\xi e^{-i\xi(t) \cdot \hat{p}} \exp \left\{ \int_0^t ds \left[i\eta(s) \cdot \dot{\xi}(s) - H_\alpha(\eta(s), \hat{q} + \xi(s)) \right] \right\}. \quad (44)$$

This expression is interpreted as a formal integral over all paths $s \mapsto (\eta(s), \xi(s))$ in phase-space $\mathbb{R}^d \times \mathbb{R}^d$ with $\xi(0) = 0$. The subscript α attached to the integration sign reminds that it is essential to strictly use the α -point discretization together with the α -symbol [31, 30, 38]. Otherwise there is no guarantee that the phase-space path integral represents the given semigroup. Conversely, replacing H_α in (44) by a given classical Hamilton function H leads to the semigroup generated by the α -ordered Hamilton operator $\{H(\hat{p}, \hat{q})\}_\alpha$. In case of the standard Hamiltonian (38) the

momentum variables in (43) can be integrated out yielding a discretized expression for the Feynman–Kac– α formula (cf. (24) and (6)). Thereby one recognizes the well-known fact that the α -point discretization underlies the definition of the α -stochastic integral [33] [39, p. 136], which hence is in one-to-one correspondence with the α -ordering scheme (see also [30]). This is reflected by the conversion formula

$$\frac{1}{2} (\hat{p}g(\hat{q}) + g(\hat{q})\hat{p}) = \{\hat{p}g(\hat{q})\}_\alpha + i \left(\frac{1}{2} - \alpha\right) (\nabla \cdot g)(\hat{q}) \quad (45)$$

similar to (6).

The basic ingredient for the validity of (43) is the *generalized Lie–Trotter formula*

$$\lim_{n \rightarrow \infty} \left[\hat{F} \left(\frac{t}{n} \right) \right]^n = \exp \left\{ t \dot{\hat{F}}(0) \right\} \quad \text{if} \quad \hat{F}(0) = \hat{1}. \quad (46)$$

It can easily be verified by a Taylor expansion if $\hat{F}(t)$ acts on a finite-dimensional Hilbert space. Suitable technical assumptions for the extension to the infinite-dimensional case are specified in [11], see also [15]. The (semigroup version of the) original Lie–Trotter formula (see, e.g. [42]) corresponds to the choice $\hat{F}(t) = e^{-t\hat{A}}e^{-t\hat{B}}$ for operators \hat{A} and \hat{B} obeying suitable conditions. Nelson [36] was the first to use it explicitly in the context of path integration. Note that without the presence of the Wiener measure the application of the original Lie–Trotter formula with $\hat{A} = \hat{p}^2/2$ and $\hat{B} = v(\hat{q})$ is of much less analytical value than the standard Feynman–Kac formula (for $a = 0$). In fact, one can use the latter to prove norm-convergence in the former [23].

An interesting question is whether it is possible to construct a measure on a suitable set of paths in phase space in order to benefit from general integration theory also in the case of non-standard Hamiltonians. One possibility is offered by Wiener-regularized expressions in the spirit of [13]. Another one derives from (22) for Hamiltonians of the form $\widehat{H} = h_+(\hat{p})h_-(\hat{q}) + h_-(\hat{q})h_+(\hat{p})$. Both methods may also be used for systems with other than canonical degrees of freedom, e.g. spin systems.

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